Molecular Simulations of Ion Exchange in NaA Zeolite Membranes

S. Murad,[C, S] W. Jia and M. Krishnamurthy
Chemical Engineering Department, University of Illinois at Chicago, Chicago, IL, U.S.A.

Molecular simulations using the method of molecular dynamics have been carried out to determine the possibility of studying ion exchange between electrolyte solutions (here an aqueous LiCl solution) and an ion exchange membrane (NaA zeolite) using direct simulations of up to a nano-second. Our results show that with appropriate driving forces, such ion exchange processes can be clearly witnessed and investigated using molecular simulations. We have also attempted to understand the phenomenon at the molecular level. Our results have shown that the ion-exchange process is energetically driven and entropic forces are not playing any significant role in the exchanges observed. We observed smaller differences between the energy of the Li inside and outside the membrane, compared to the Na ions, making the exchange process energetically favorable. Simulations can also be potentially very useful to determine the behavior of hydrodynamic parameters commonly used to characterize ion-exchange processes at a fundamental molecular level, as well to determine if the hydrodynamic equations used for ion-exchange processes are applicable to nano-systems that can be studied using simulations.